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A Dissymmetric, Singly Phenoxido-bridged CuII Dinuclear Coordination  
Compound: Synthesis, Characterization, Magnetic and Computational  
Study

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Abstract

A singly phenoxido-bridged dinuclear Cu<sup>II</sup> complex, [Cu<sub>2</sub>(L)<sub>2</sub>(SCN)<sub>2</sub>(H<sub>2</sub>O)], has been obtained from a Schiff-base ligand (2-[{2-(dimethylamino)ethyl}imino}methyl]-6-methoxyphenol), generated by condensation of *o*-vanillin with *N,N*-dimethylethane-1,2-diamine. The Cu(II) complex has been fully characterised by analytical, spectroscopic, magnetic susceptibility and EPR measurements and DFT calculations, as well as single-crystal X-ray diffraction analysis. It consists of two geometrically distinct square-pyramidal and octahedral copper(II) centres, exhibiting N<sub>2</sub>O<sub>3</sub> and N<sub>4</sub>O<sub>2</sub> donor sets. In the dimeric unit, the copper atoms are connected by a  $\mu_2$ -phenolato oxygen atom, belonging to one bridging Schiff-base ligand. Variable-temperature magnetic susceptibility measurements indicate strong antiferromagnetic exchange interactions between the Cu(II) centres, with a  $2J$  value of  $-89(1) \text{ cm}^{-1}$ .

Key words : COPPER(II); PHENOXIDO-BRIDGE; SPECTROSCOPIC  
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